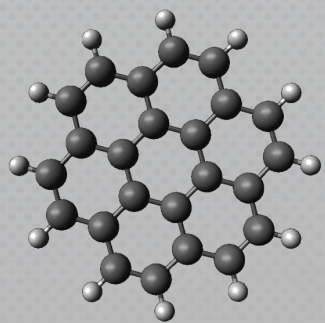
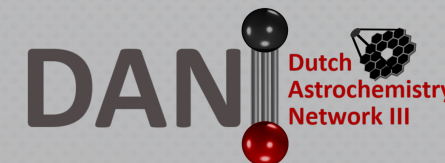


The Aromatic Cosmos: exploring Carbon chemistry in space



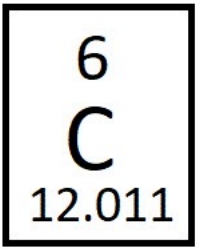
Alessandra Candian
Anton Pannekoek Institute
University of Amsterdam

FIR 2025, 2-5 April 2025, Leiden

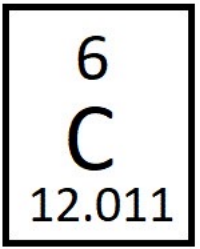


Cosmic Carbon

- 4th most abundant element in the Universe

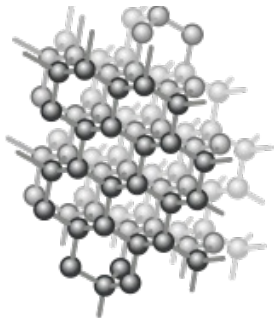


Cosmic Carbon

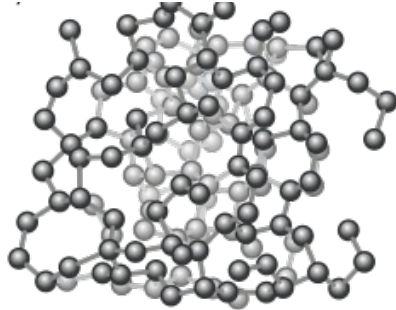


- 4th most abundant element in the Universe
- Different “shapes” => building block of life as we know it

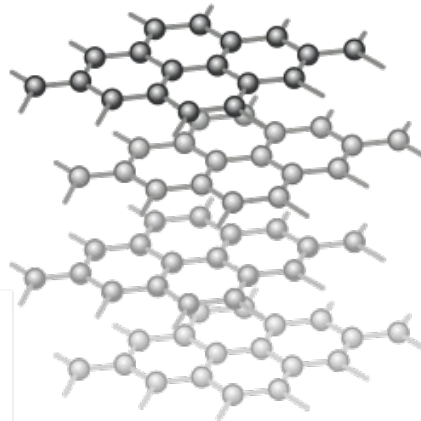
diamond



amorphous carbon

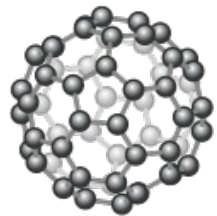


graphite

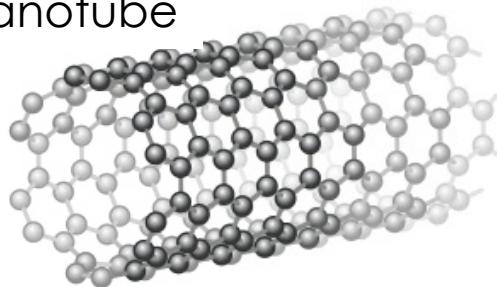


● C

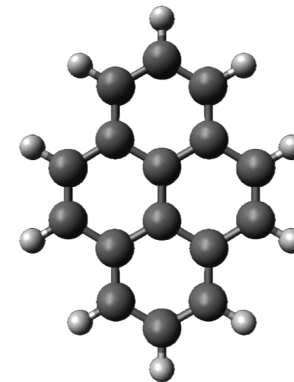
fullerene



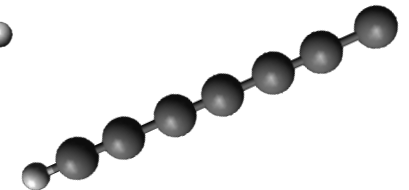
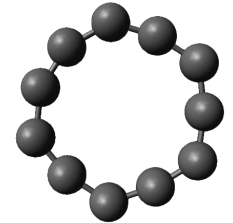
nanotube



PAHs



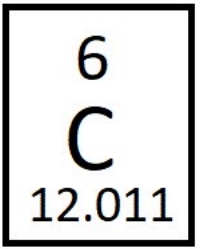
carbon cluster



carbon chain

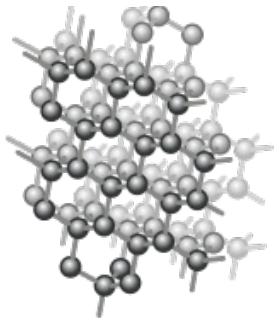
Jozef Sivek, CC-BY-SA 4.0

Cosmic Carbon

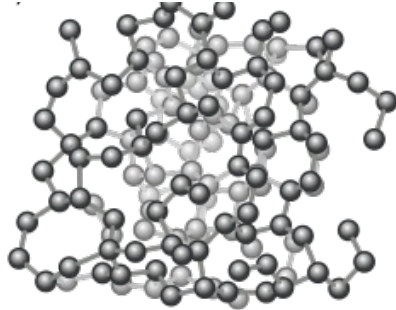


- 4th most abundant element in the Universe
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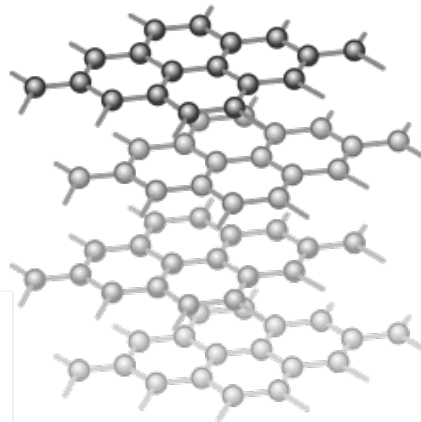
diamond



amorphous carbon

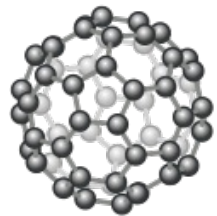


graphite

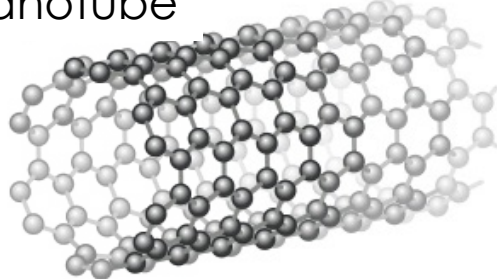


● C

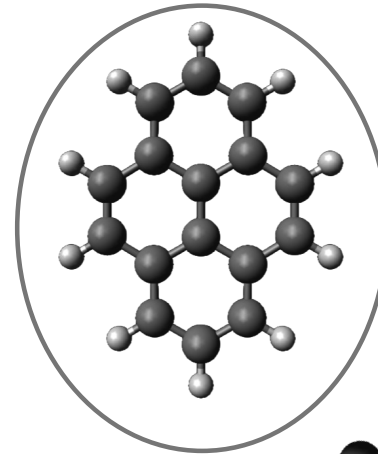
fullerene



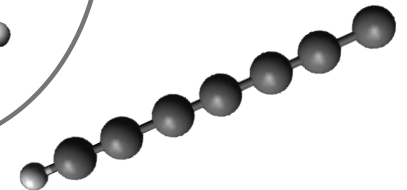
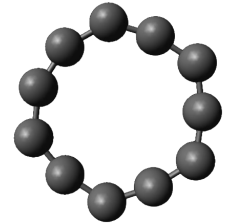
nanotube



PAHs

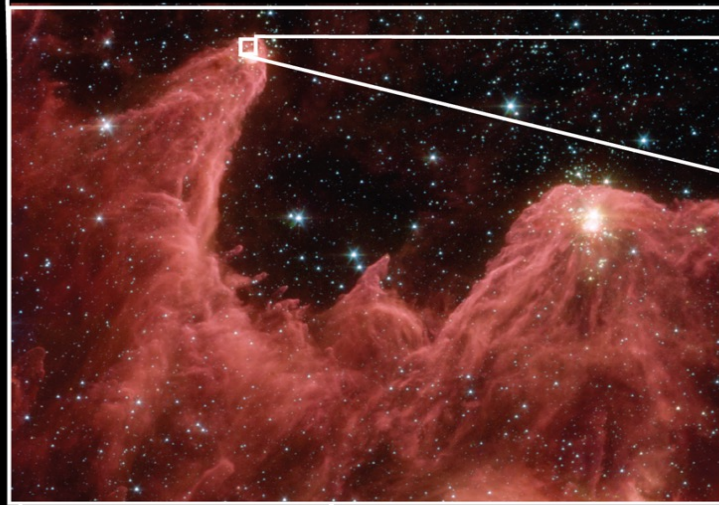


carbon cluster

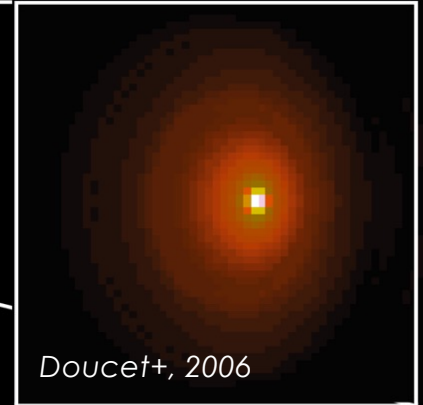


carbon chain

Jozef Sivek, CC-BY-SA 4.0



HD 97048



Doucet+, 2006

Star-forming regions

PAHs are **STRONG & UBIQUITOUS**

~20% of the IR flux in galaxies & 10% of cosmic Carbon (Tielens 2008)

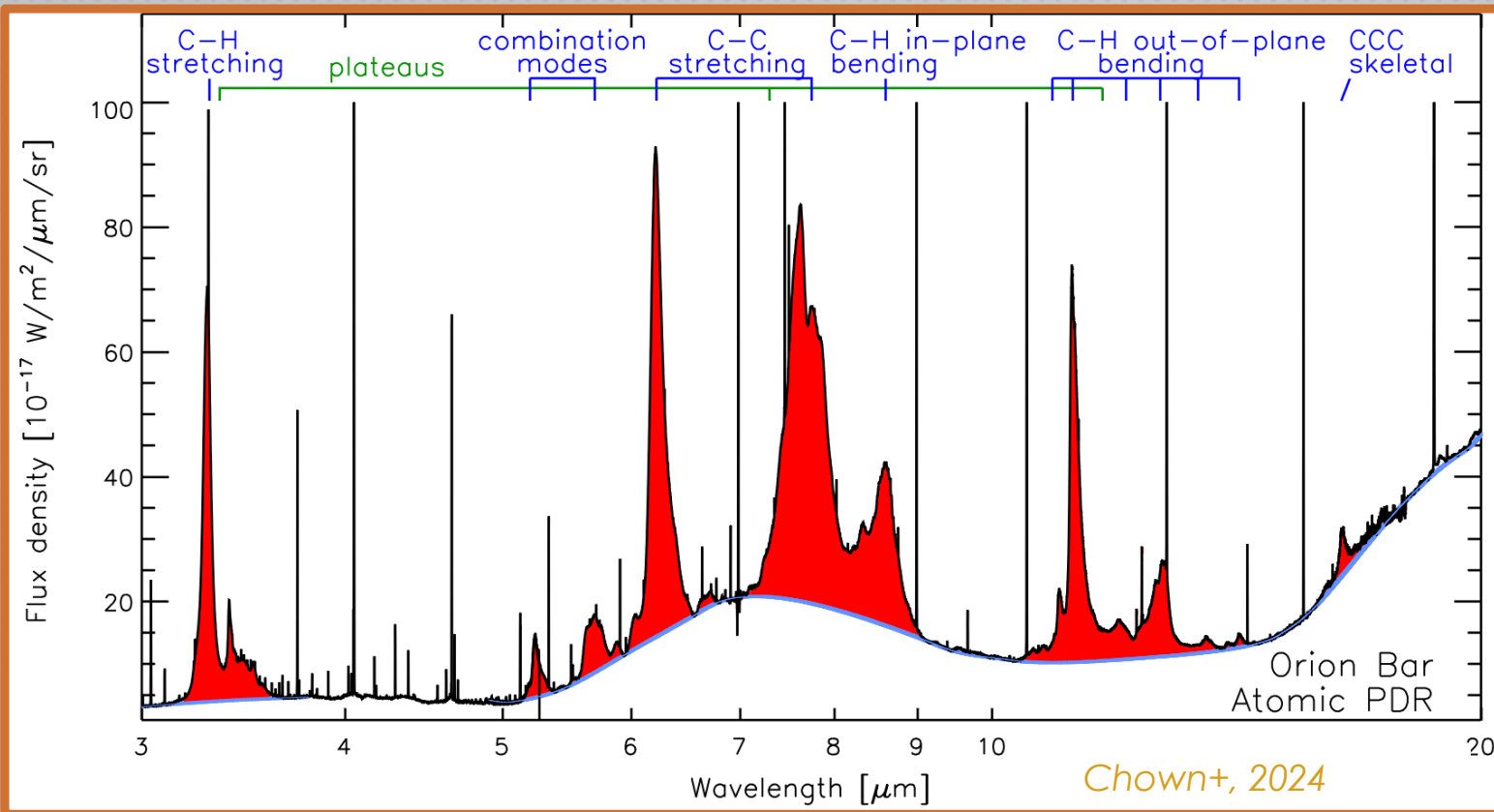
- In galaxies up to $z \sim 4$ (Rigopoulou+ 2024, Spilker+2023, Chen+, 2024)
- In the Solar system (Lopez-Puertas+, 2013; Vinatier+ 2012; Clemett+2010; Li, 2008)

Perfect TEST molecules to trace the Carbon lifecycle in the ISM



M481

PAHs and Aromatic Infrared Bands



JWST launch gives a new view on PAH emission



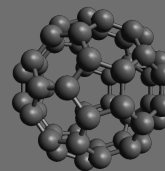
A Population of AstroPAH

Several IR mission and the interdisciplinary work of astronomers, experimentalist and theoreticians put constraints on Astro PAH population

Charge:
+/0/-

Size:
 $N_C > 50$

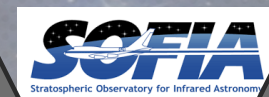
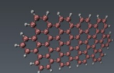
C_{60}



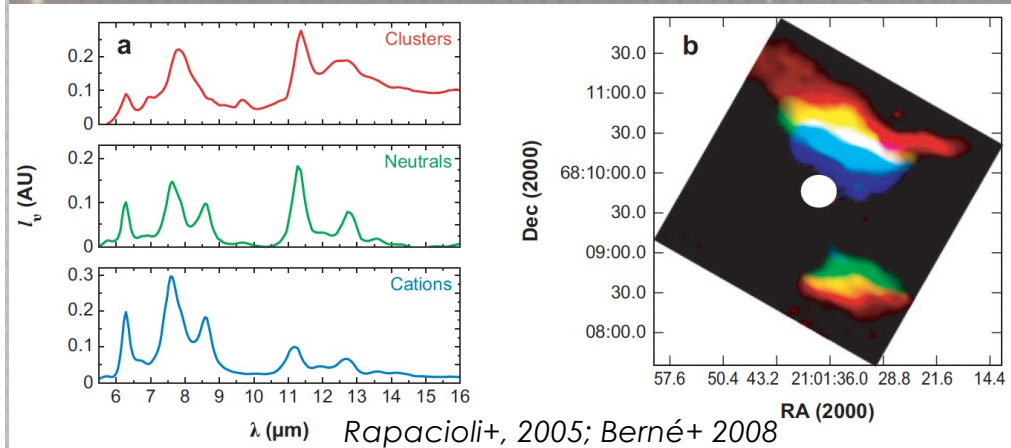
Funct.
groups:
 CH_3 , CN

Hetero
atoms:
D, O

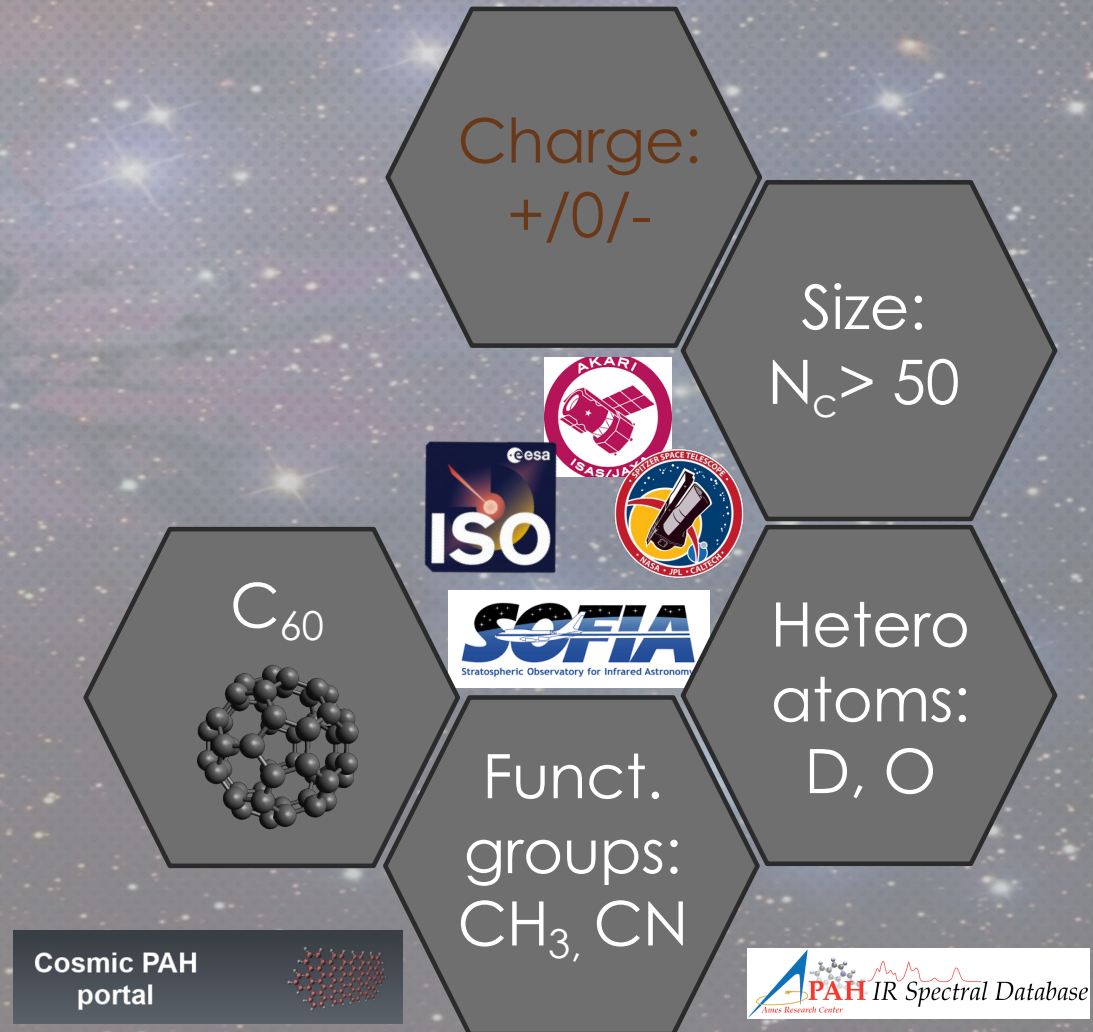
Cosmic PAH
portal



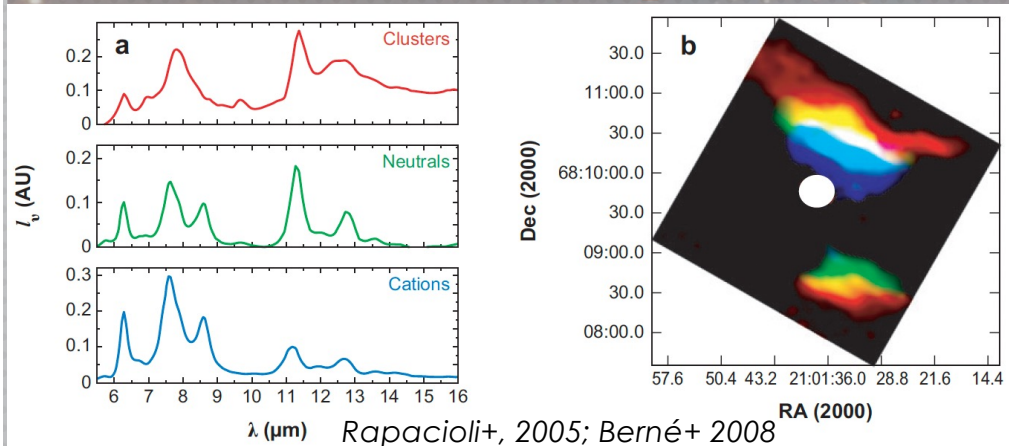
A Population of AstroPAH



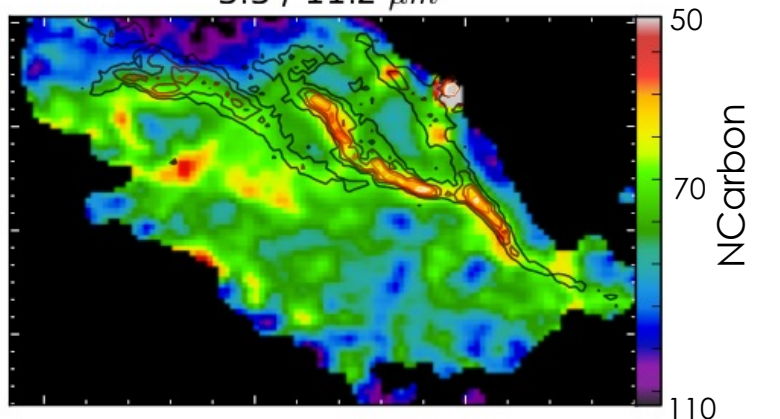
Charge PAHs dominate close to the central star



A Population of AstroPAH



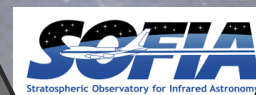
3.3 / 11.2 μm Croiset+, 2016



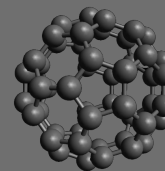
We can trace the PAH size using band ratios.

Charge:
+/0/-

Size:
 $N_C > 50$



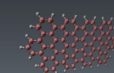
C_{60}



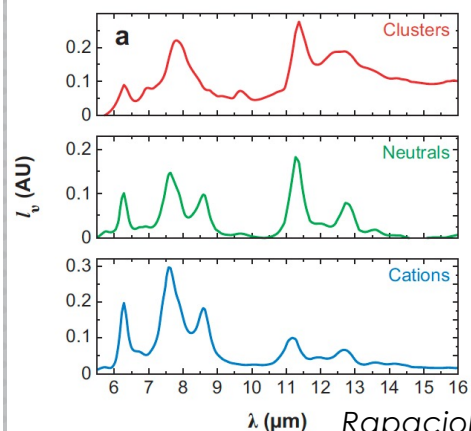
Hetero
atoms:
D, O

Funct.
groups:
 CH_3 , CN

Cosmic PAH
portal

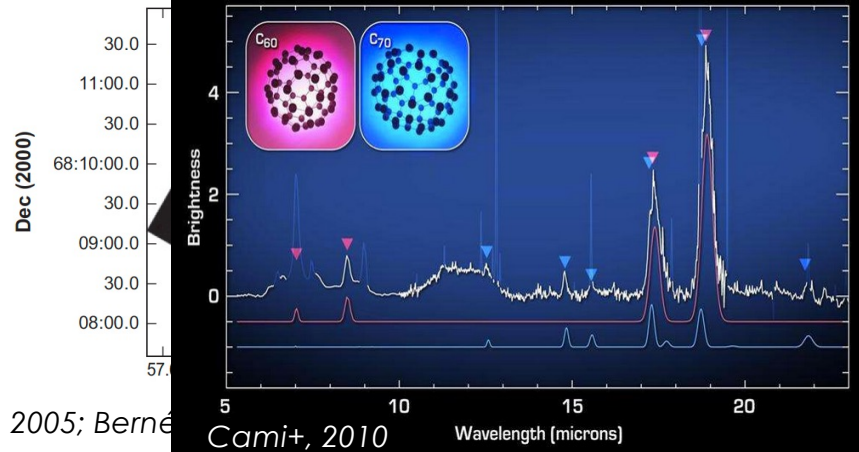
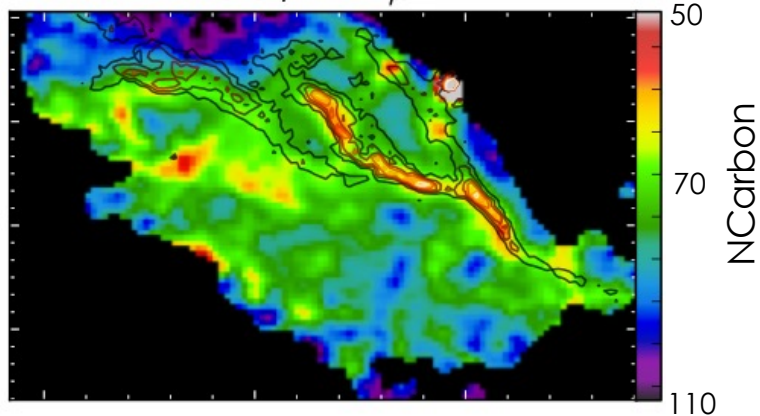


A Population of AstroPAH



λ (μm) Rapacioli+, 2005; Berné

3.3 / 11.2 μm Croiset+, 2016



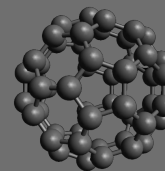
Charge:
+/0/-

Size:
 $N_c > 50$



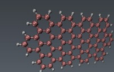
Hetero
atoms:
D, O

C_{60}



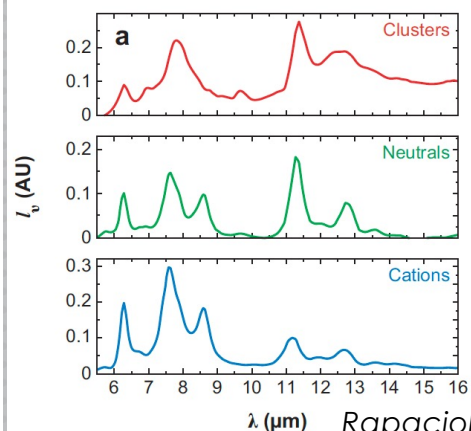
Funct.
groups:
 CH_3 , CN

Cosmic PAH
portal



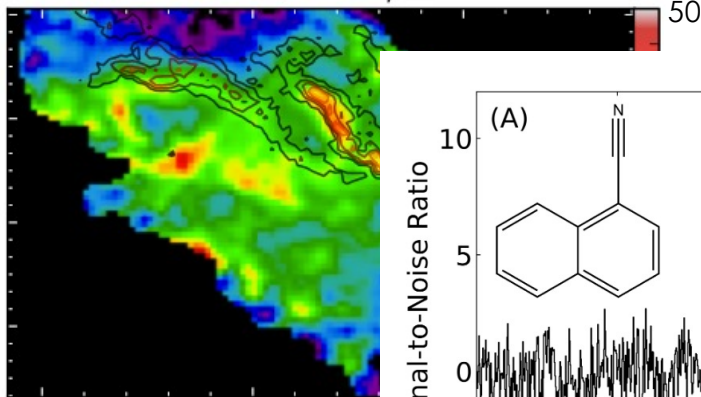
PAH IR Spectral Database
Ames Research Center

A Population of AstroPAH

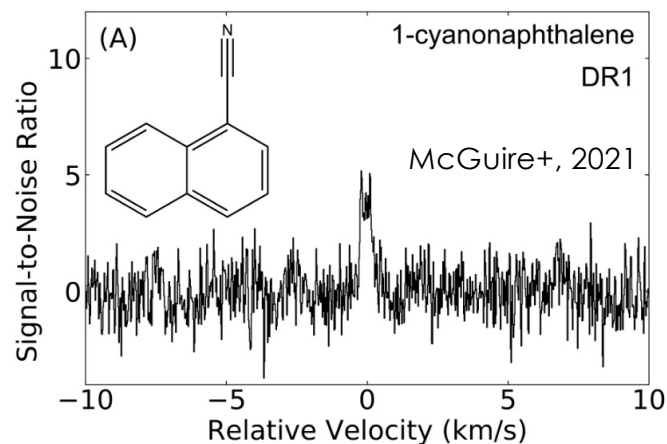
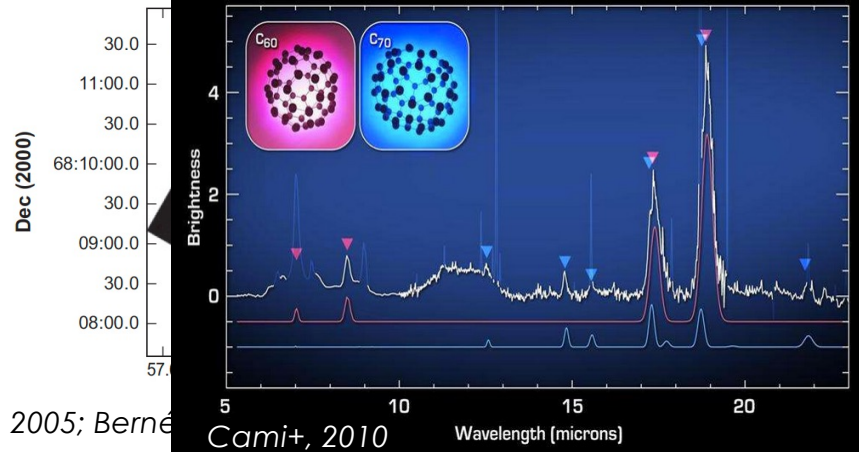


λ (μm) Rapacioli+, 2005; Berné

3.3 / 11.2 μm Croiset+, 2016



Cernicharo+, 2024
Wenzel+, 2025

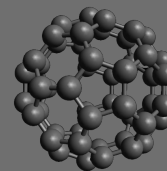


Charge:
+ / 0 / -

Size:
 $N_C > 50$



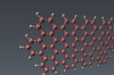
C_{60}



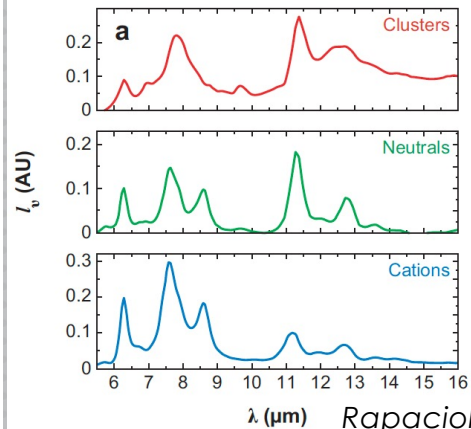
Hetero
atoms:
D, O

Funct.
groups:
 CH_3 , CN

Cosmic PAH
portal

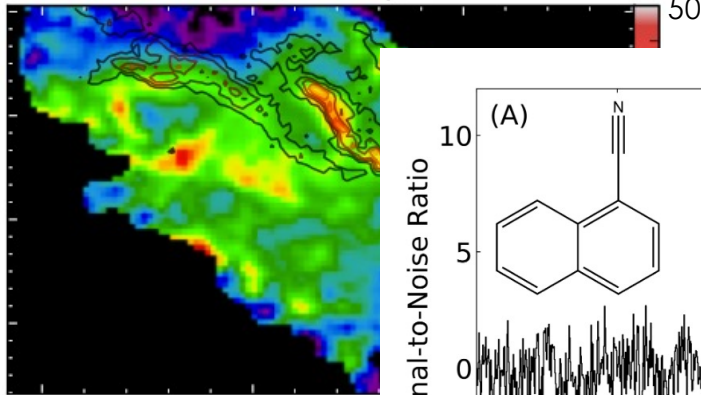


A Population of AstroPAH

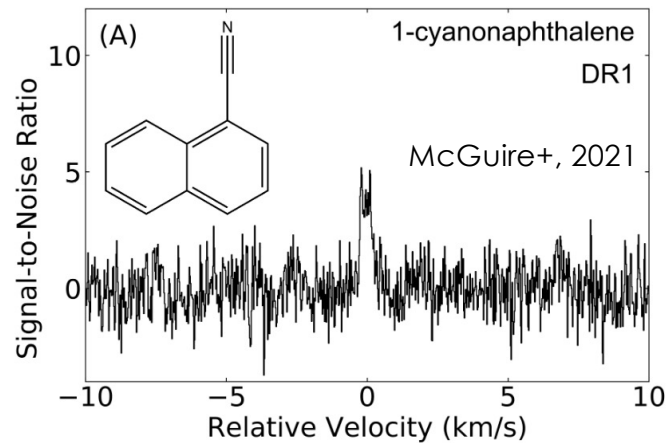
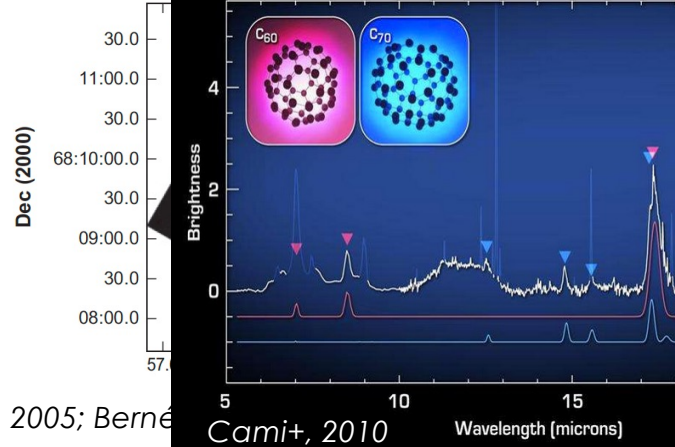


Rapacioli+, 2005; Berné

3.3 / 11.2 μm Croiset+, 2016



Cernicharo+, 2024
Wenzel+, 2025



Cosm
p

Ames Research Center

se



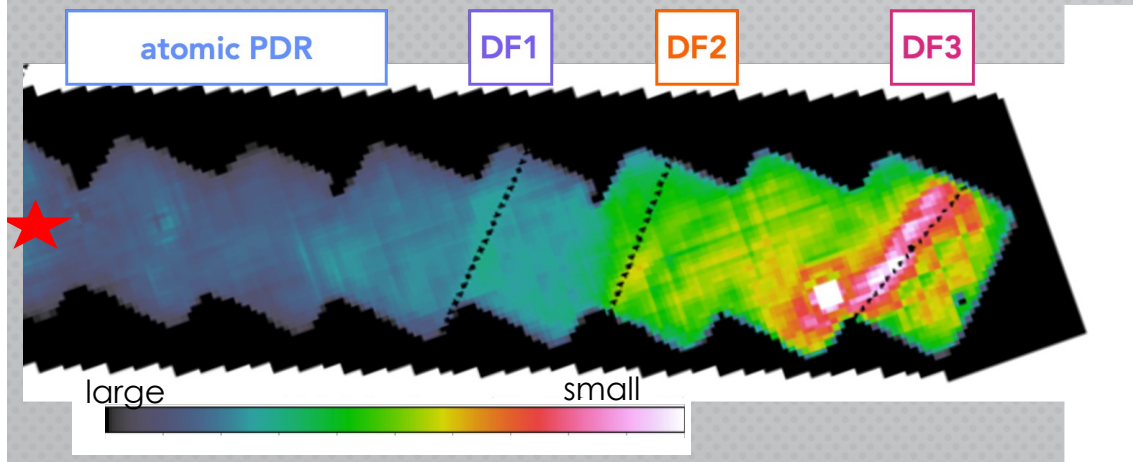
The evolution of AstroPAHs: JWST

PI: Berné, Habart and Peeters



The evolution of AstroPAHs: JWST

PI: Berné, Habart and Peeters



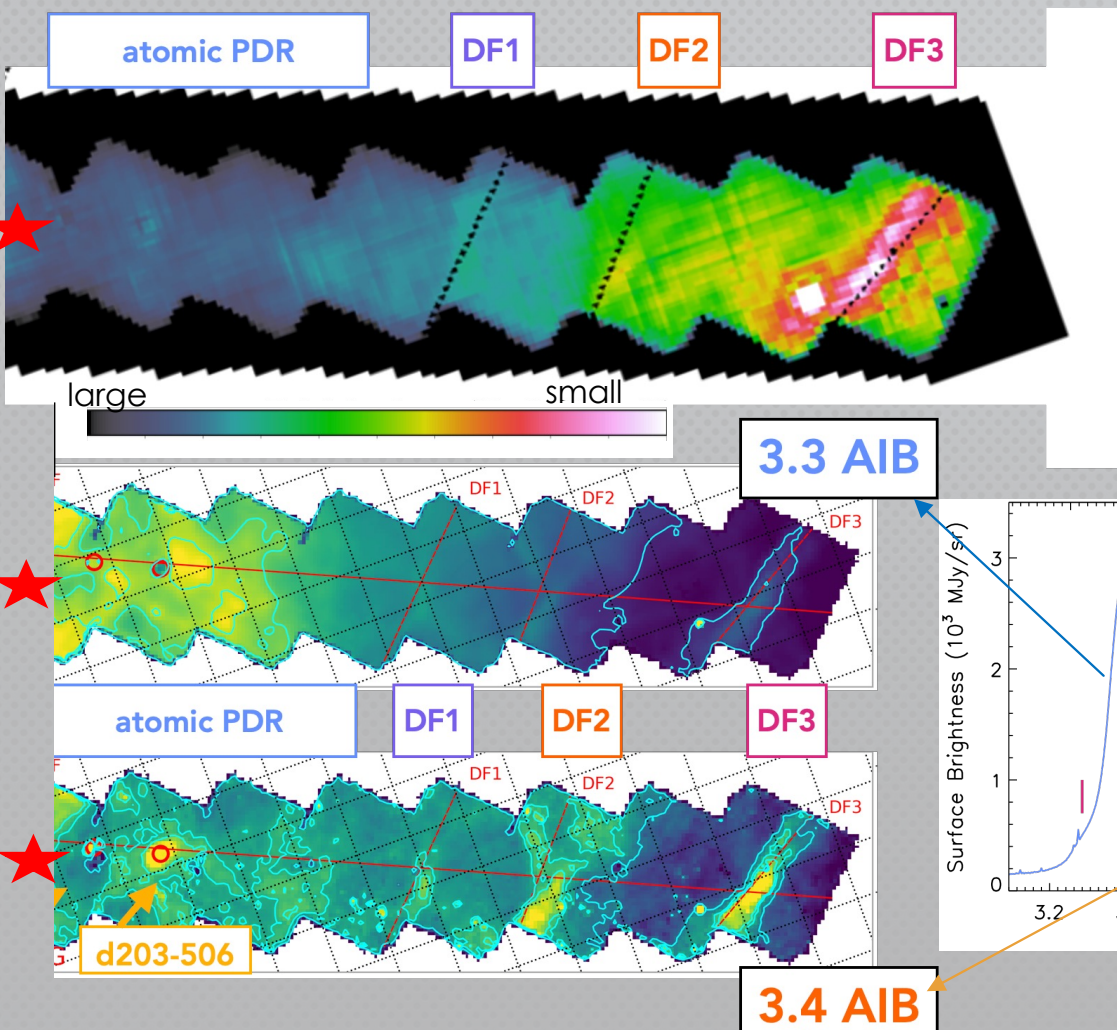
PAH SIZE: 3.3/11.2 ratio

- Larger PAHs closer to the PDR surface
- Smaller PAHs in the more shielded environment



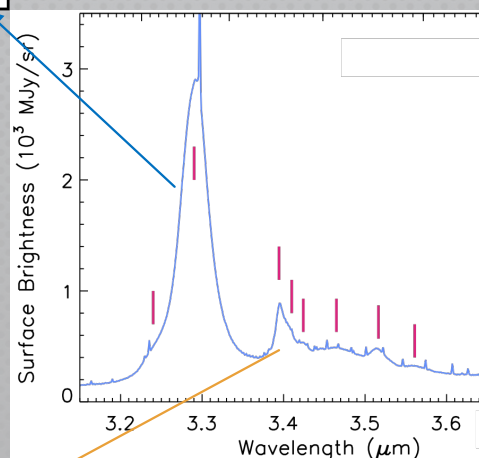
The evolution of AstroPAHs: JWST

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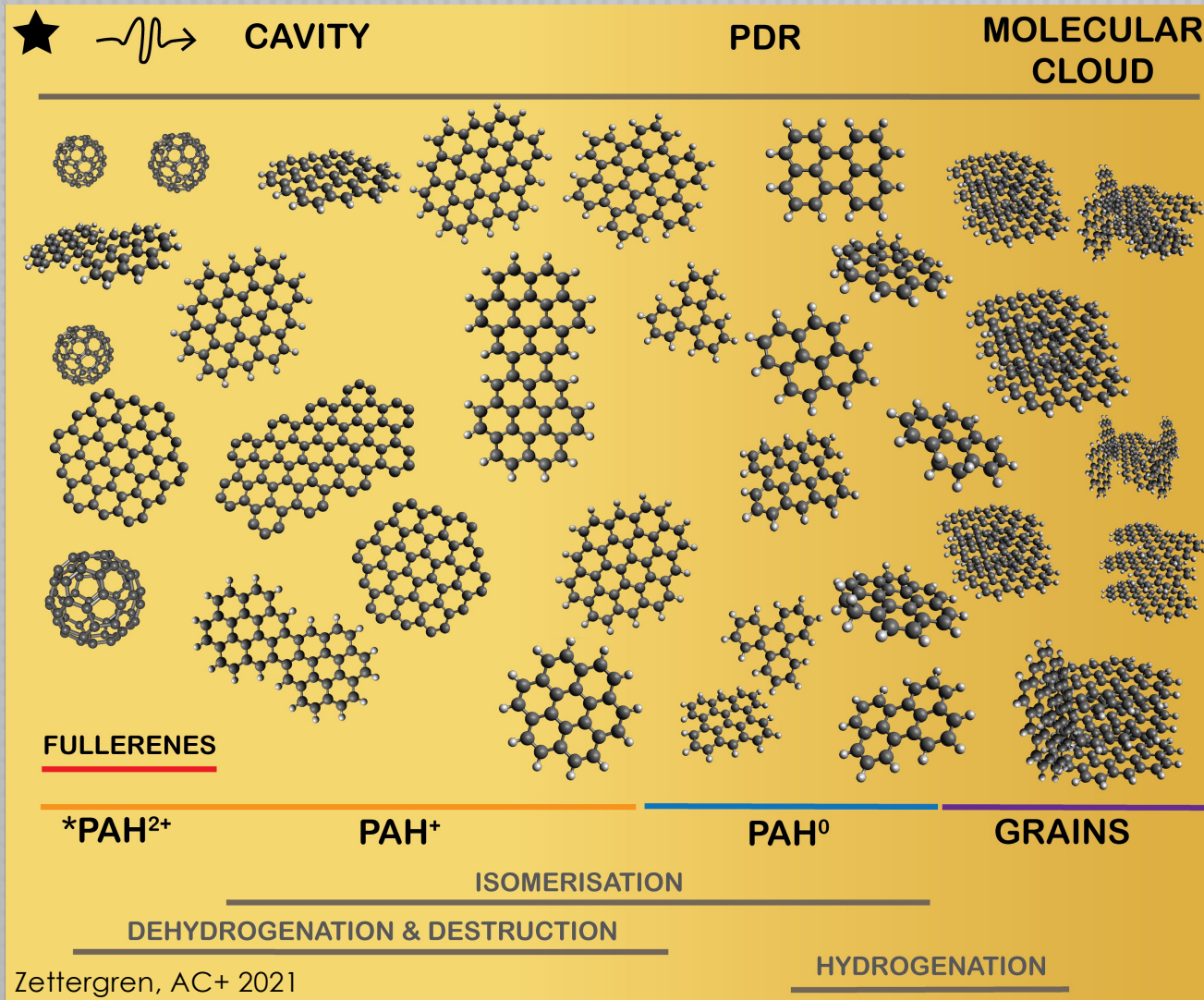


Aliphatic (3.4)/Aromatic (3.3) ratio

- Aliphatic sidegroups destroyed by UV field

Chown+, 2024; Scheffer+, in prep

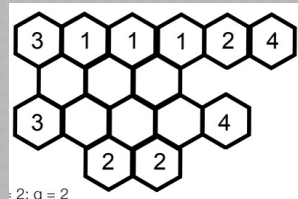
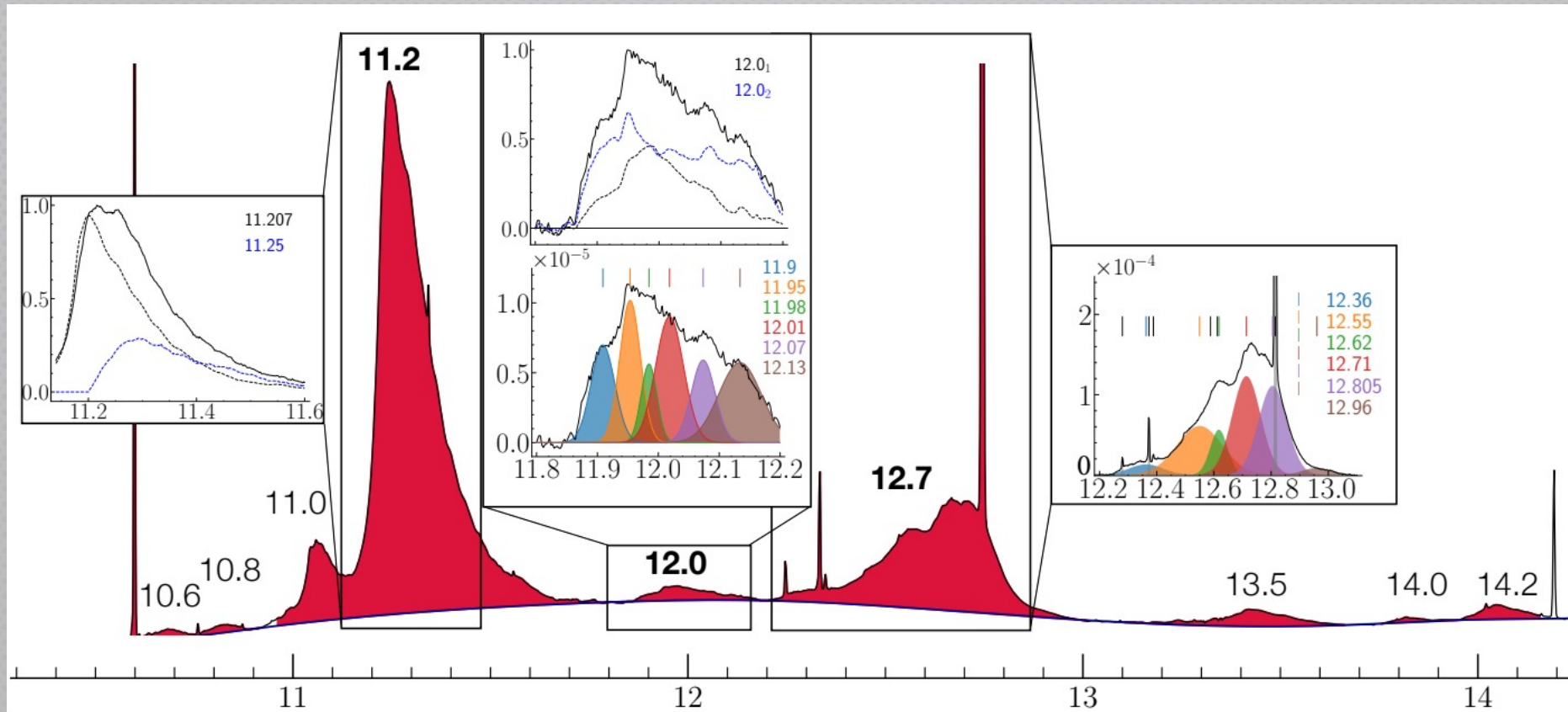
PAH photochemical evolution



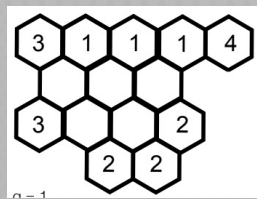
Supported by experiments and modelling

(Berne and Tielens 2010; Montillaud+, 2014, 2016; Castellanos, AC, +, 2018a, b; Andrews, AC, + 2016, Panchagnula, Kamer, AC et al., 2024; Sundararajan, AC et al., 2024)

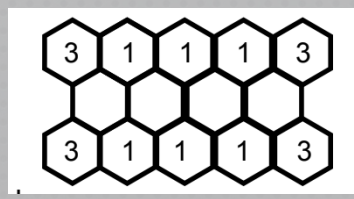
The shape of AstroPAHs: JWST



2; q=2



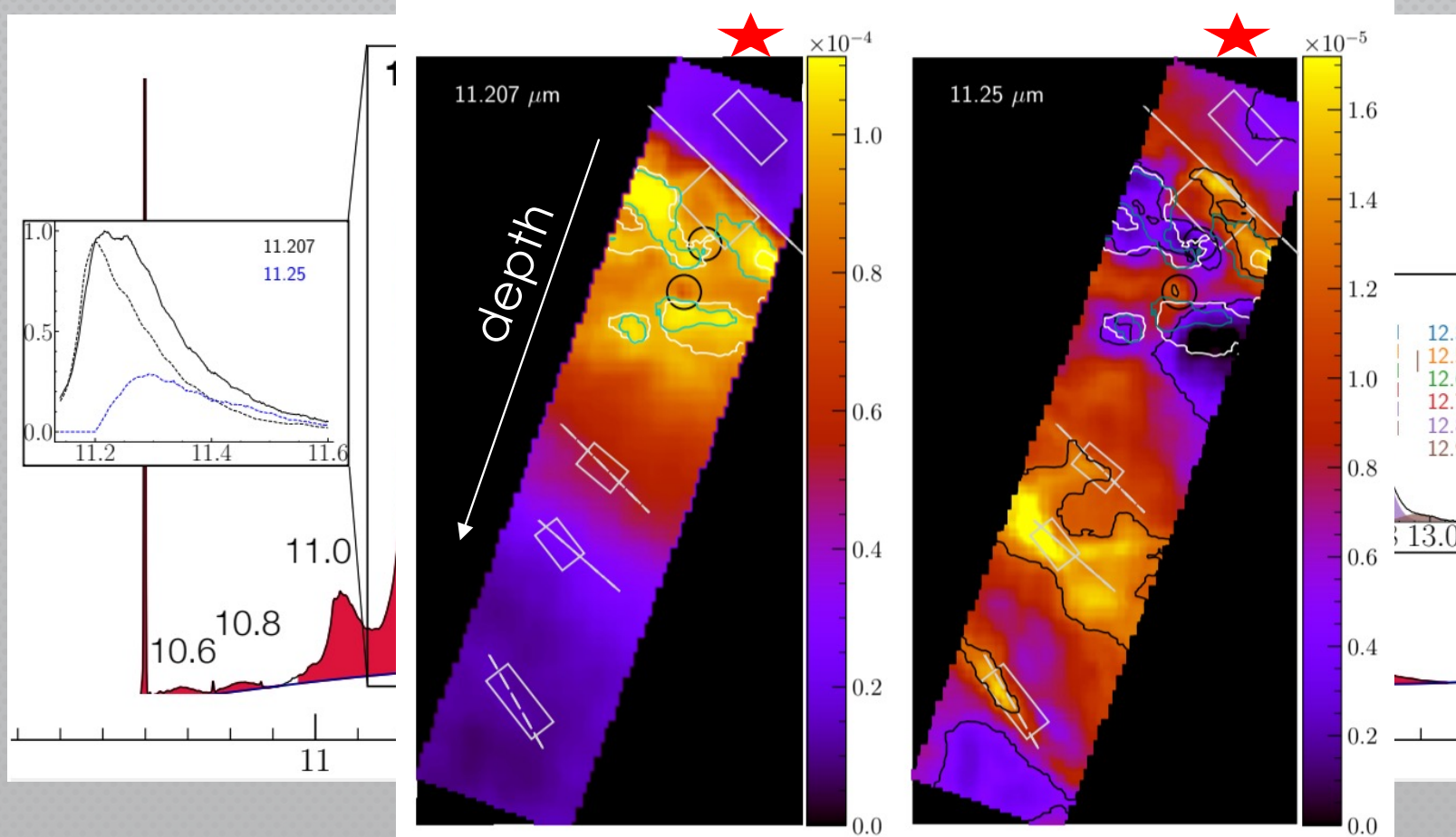
q=1



Possible PAH shapes proposed for the Orion Bar

Khan+, 2025

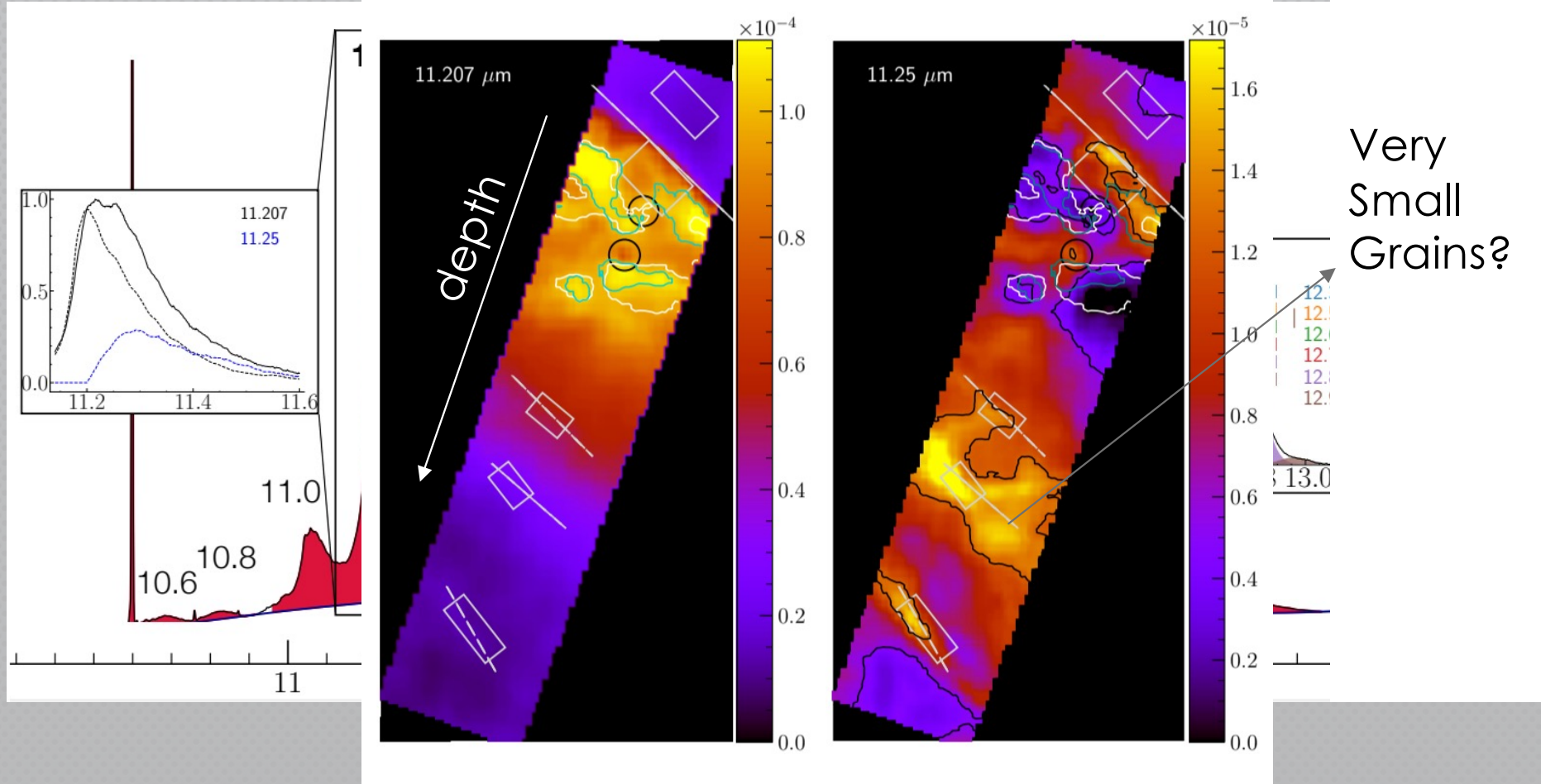
The shape of AstroPAHs: JWST



11.2 μm has 2 components with different spatial distribution

Khan+, 2025

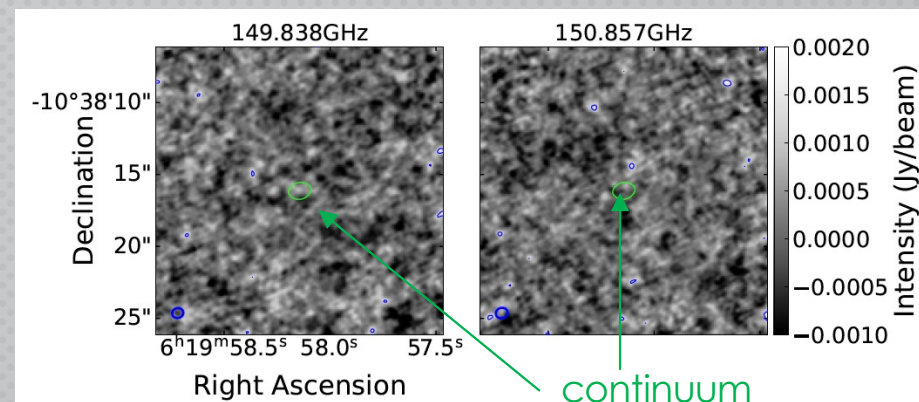
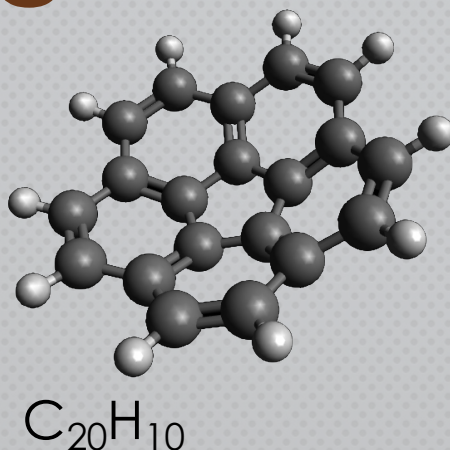
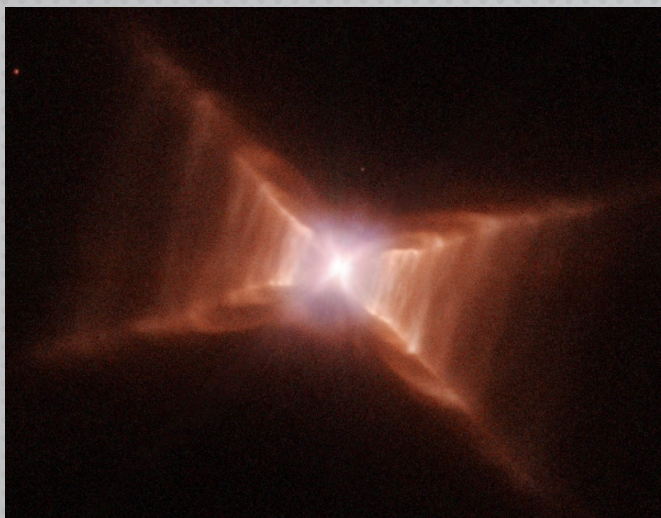
The shape of AstroPAHs



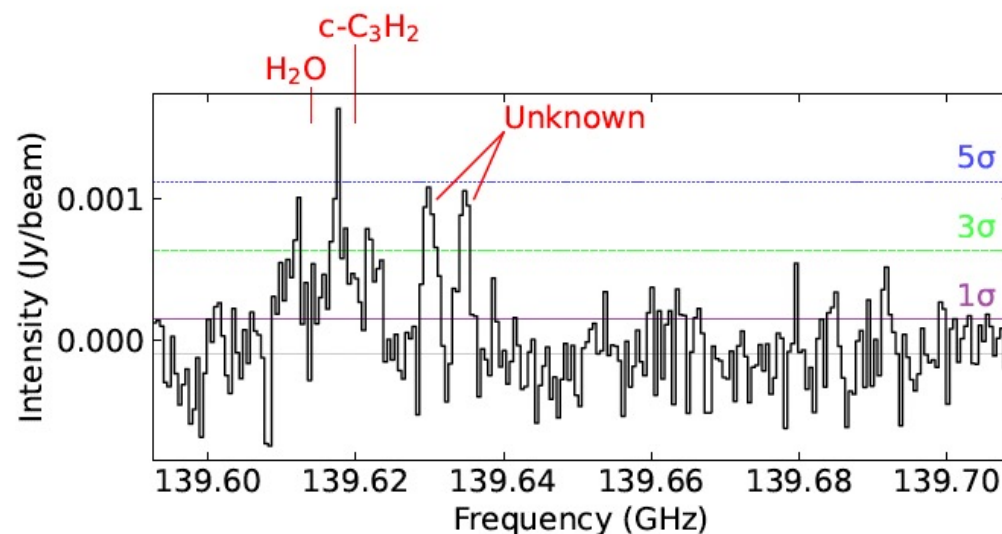
11.2 μm has 2 components with different spatial distribution

Khan+, 2025

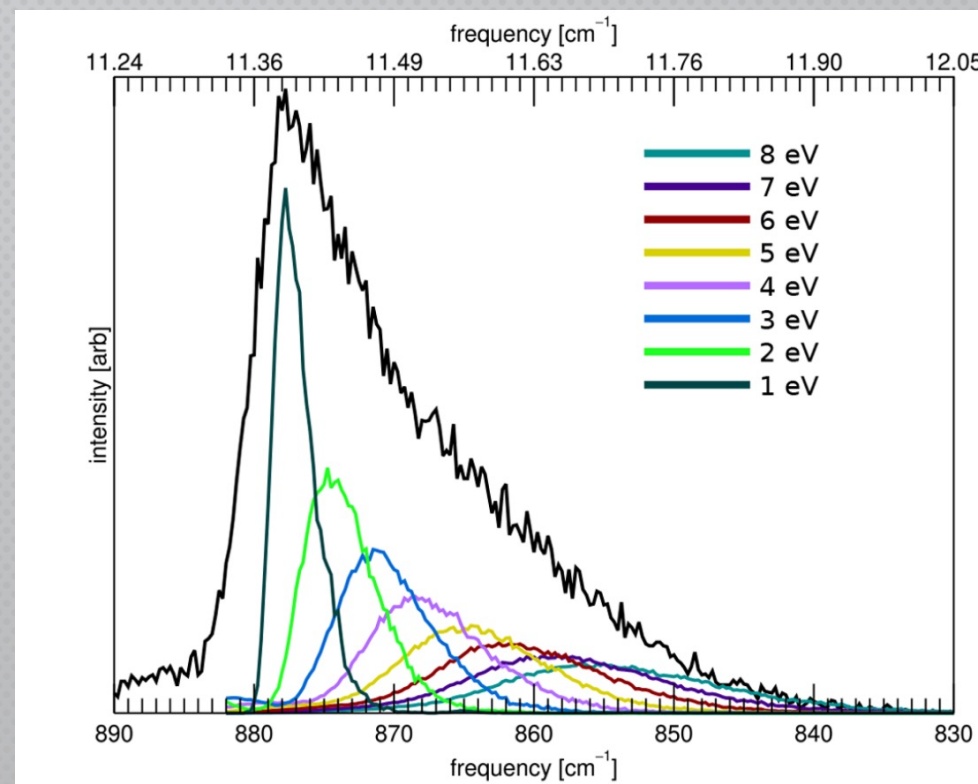
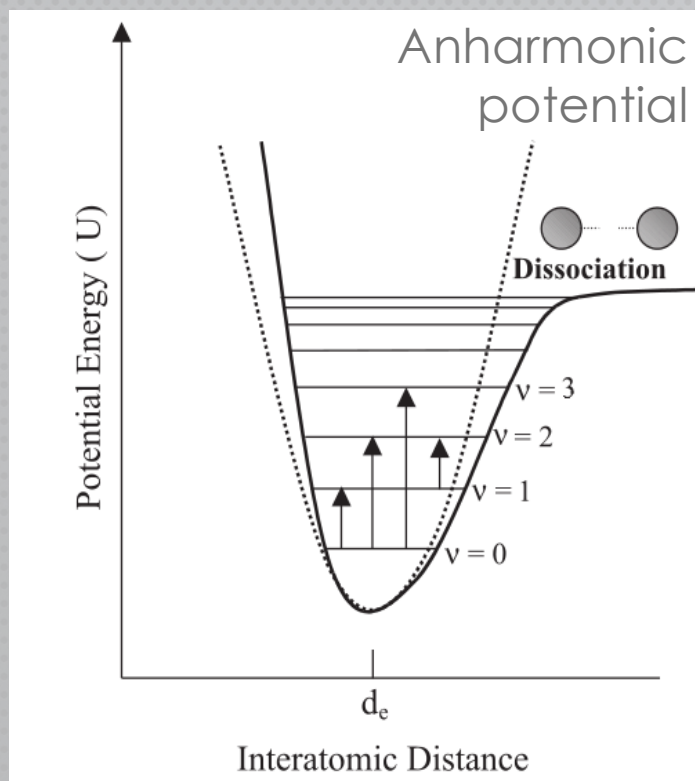
Searching for PAHs with ALMA



- 9hrs ALMA observations
- Upper limit nC in corannulene: 9×10^{-7}
- Revising formation routes
- Tentative detection of H_2O and $c-C_3H_2$: mini-PDR region? (Bujarrabal+, 2023)



Improving PAH spectral modelling

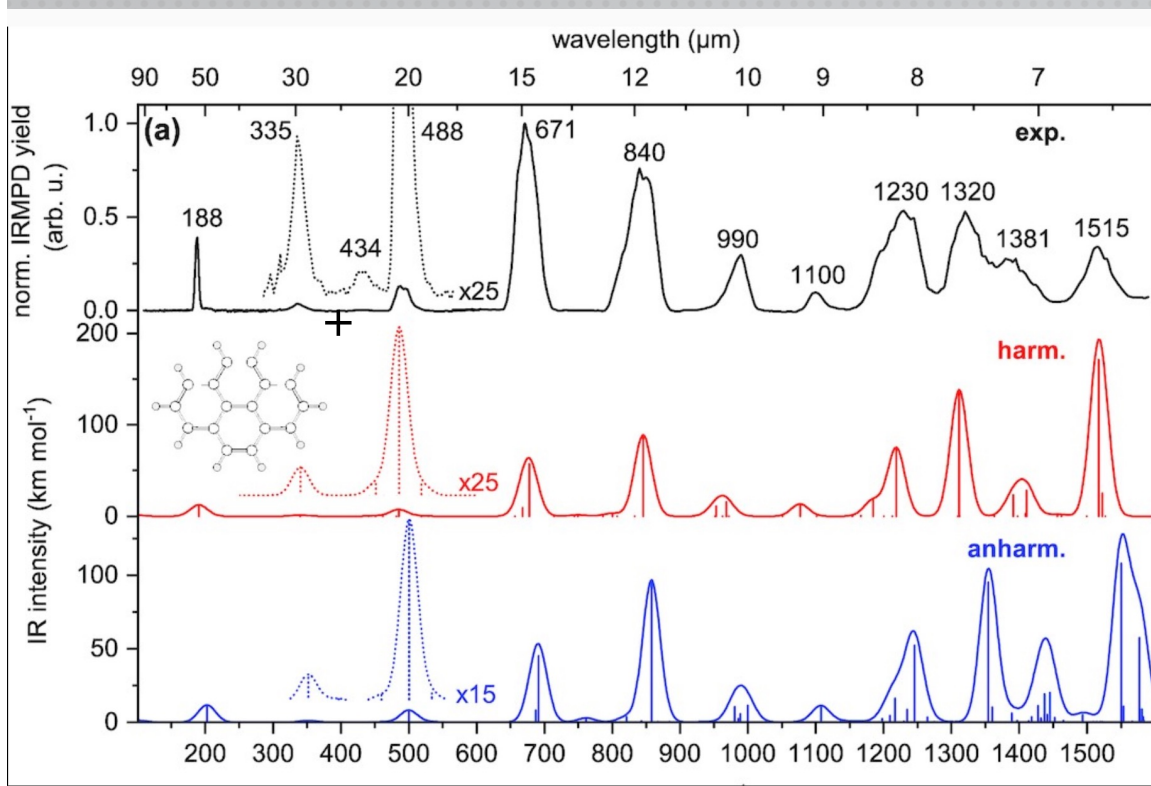


Accurate Quantum Chemistry calculations + benchmark with experiments to obtain “real” PAH emission spectrum

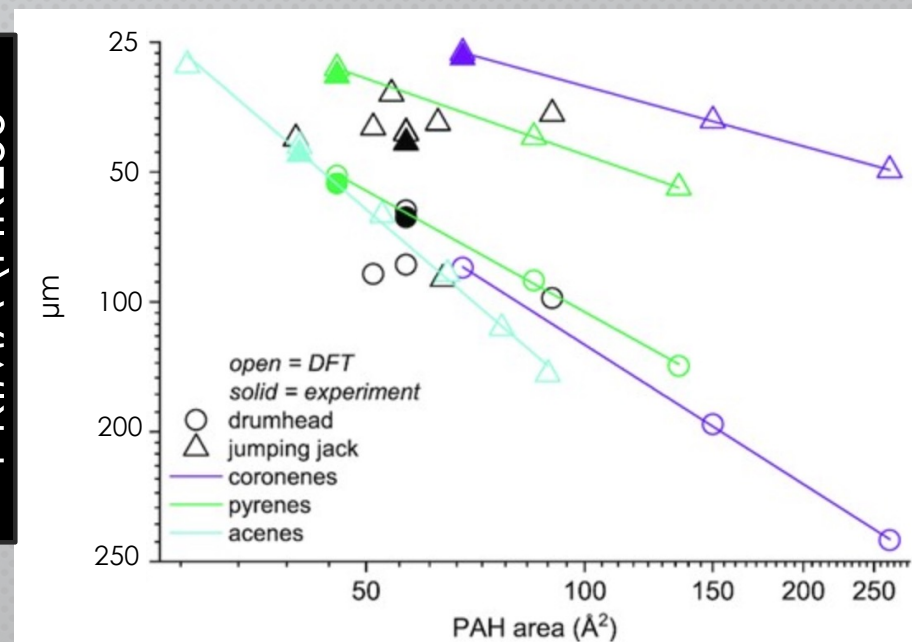
Mackie, AC+ 2021; Peeters+ 2021; Reems, AC + in prep.

PAHs FAR-IR modes and PRIMA

Joblin et al 2011; Wiersma, AC, et al 2022



PRIMA\FIRESS



PAHs have intense far-IR very harmonic vibrational modes => FIRESS can “identify” PAHs in irradiated regions because modes are symmetry-dependent

Take home message

- PAHS ARE FUNDAMENTAL INGREDIENTS OF THE ISM
- JWST ALLOWS US TO CONSTRAIN PAH EVOLUTION FROM THE ISM TO PLANET-FORMING REGIONS
- EXPERIMENTS, COMPUTATIONAL CHEMISTRY AND MODELLING ARE FUNDAMENTAL TO INTERPRET OBSERVATIONS
- FIRESS COULD IDENTIFY PAHS IN PDRs

